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# Logarithmic Corrections to Scaling in the Two Dimensional $XY$ -Model

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## **Abstract**

By expressing thermodynamic functions in terms of the edge and density of Lee–Yang zeroes, we relate the scaling behaviour of the specific heat to that of the zero field magnetic susceptibility in the thermodynamic limit of the  $XY$ -model in two dimensions. Assuming that finite-size scaling holds, we show that the conventional Kosterlitz–Thouless scaling predictions for these thermodynamic functions are not mutually compatible unless they are modified by multiplicative logarithmic corrections. We identify these logarithmic corrections analytically in the case of the specific heat and numerically in the case of the susceptibility. The techniques presented here are general and can be used to check the compatibility of scaling behaviour of odd and even thermodynamic functions in other models too.

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**The Kosterlitz–Thouless Scenario** The partition function for the  $O(n)$  non-linear  $\sigma$ -model defined on a regular  $d$ -dimensional lattice  $\Lambda$  with periodic boundary conditions in the presence of an external magnetic field can be written as

$$Z_L(\beta, h) = \frac{1}{\mathcal{N}} \sum_{\{\vec{\sigma}_x\}} e^{\beta S + h \vec{n} \cdot \vec{M}}, \quad (1)$$

where  $\vec{n}$  is a unit vector defining the direction of the external magnetic field and  $h$  is a scalar parameter representing its strength. The summation is over all configurations open to the system. The factor  $\mathcal{N}$  ensures that  $Z_L(0, 0) = 1$  and

$$S = \sum_{x \in \Lambda} \sum_{\mu=1}^d \vec{\sigma}_x \cdot \vec{\sigma}_{x+\mu}, \quad \vec{M} = \sum_{x \in \Lambda} \vec{\sigma}_x.$$

Here  $L$  represents the linear extent of the system,  $\beta = 1/kT$  and  $\vec{\sigma}_x$  is an  $n$ -component unit length spin at site  $x \in \Lambda$ . The case  $d = 2$ ,  $n = 2$  is the two dimensional  $XY$ -model or plane rotator model and is unusual in that it exhibits an exponential singularity. Using an approximate renormalization group approach, Kosterlitz and Thouless [1] demonstrated the existence of a phase transition driven by the condensation of vortices. The model remains critical (thermodynamic functions diverge) for all  $\beta > \beta_c$  and the critical exponents are dependent on temperature. In terms of the reduced temperature

$$t = 1 - \frac{\beta}{\beta_c},$$

the scaling behaviour of the correlation length, susceptibility and the specific heat is given in [1] as

$$\xi_\infty(t) \sim e^{at^{-\nu}}, \quad (2)$$

$$\chi_\infty(t) \sim \xi_\infty^{2-\eta}, \quad (3)$$

$$C_\infty(t) \sim \xi_\infty^{\tilde{\alpha}} + \text{constant}, \quad (4)$$

where for  $t \rightarrow 0^+$ ,  $\nu = 1/2$ ,  $\eta = 1/4$  and  $\tilde{\alpha} = -d = -2$ . The purpose of this work is to argue that the latter two scaling formulae are incompatible as they stand. To this end, a method is presented by which odd and even thermodynamic functions (the susceptibility and specific heat) can be related and expressed in terms of partition function zeroes. Using certain reasonable assumptions regarding finite-size scaling, it is shown that there have to exist multiplicative logarithmic corrections <sup>2</sup> to (3) and (4). This method can be applied to any model.

**Partition Function Zeroes** Lee and Yang [2] showed the connection between critical behaviour and partition function zeroes. For a finite system these are strictly complex (non-real). As  $L \rightarrow \infty$  one expects the zeroes to condense onto smooth curves. Zeroes in the plane of complex external magnetic field  $h$  are referred to as Lee–Yang zeroes. Lee and Yang further showed that for certain systems these zeroes are in fact restricted to the imaginary  $h$  axis (the Lee–Yang theorem) [2]. In the symmetric phase,  $t > 0$ , they lie away from the real  $h$ -axis, pinching it only as  $t \rightarrow 0^+$  (in the

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<sup>2</sup>The work of [1] contains implicitly a prediction for logarithmic corrections but this seems not to have been followed up quantitatively.

thermodynamic limit). For systems obeying the Lee–Yang theorem, such as the XY Model [3], this pinching occurs at  $h = 0$  prohibiting analytic continuation from  $\text{Re}(h) < 0$  to  $\text{Re}(h) > 0$ . This means that (for the finite-size system or in the thermodynamic limit) the partition function is an entire function of  $h$  all of whose zeroes are purely imaginary. The zeroes in the complex fugacity plane ( $z \equiv \exp(h)$ ) are distributed on the unit circle. Writing these zeroes as

$$z_j(\beta) = e^{i\theta_j(\beta)},$$

the partition function is

$$Z_L(\beta, h) = \rho_L(\beta, h) \prod_j (z - e^{i\theta_j(\beta)}), \quad (5)$$

where  $\rho_L$  is a non-vanishing function of  $h$  related to the spectral density (ignored in what follows since it contributes only to the regular part of the free energy in the thermodynamic limit). The free energy is then

$$f_L(\beta, h) = L^{-d} \sum_j \ln(z - e^{i\theta_j(\beta)}). \quad (6)$$

Define the density of zeroes to be [4, 5]

$$g_L(\beta, \theta) = L^{-d} \sum_j \delta(\theta - \theta_j(\beta)) = \frac{\partial G_L(\beta, \theta)}{\partial \theta}. \quad (7)$$

Here  $G_L(\beta, \theta)$  is the cumulative density of zeroes and monotonically increases from  $G_L(\beta, 0) = 0$  to  $G_L(\beta, \pi) = 1/2$ . The distribution of zeroes is symmetric about the real  $h$ - (or  $z$ -) axis and so

$$g_L(\beta, -\theta) = g_L(\beta, \theta). \quad (8)$$

In terms of the density of zeroes, (6) becomes

$$f_L(\beta, h) = \frac{1}{2}(h + \ln 2) + \int_0^\pi \ln(\cosh h - \cos \theta) dG_L(\beta, \theta), \quad (9)$$

where (8) has been used.

In the high temperature phase there exists a region around  $\theta = 0$  which is free from Lee–Yang zeroes [2]. We define the corresponding Yang–Lee edge  $\theta_{\text{YL}}(\beta)$  by

$$g(\beta, \theta) = 0 \quad \text{for} \quad -\theta_{\text{YL}}(\beta) < \theta < \theta_{\text{YL}}(\beta).$$

The integral in (9) can therefore be taken to begin at  $\theta_{\text{YL}}(\beta)$ . Salmhofer has proved the existence of a unique density of zeroes in the thermodynamic limit [5]. In this limit, integrating (9) by parts and expanding the trigonometric functions gives for the singular part of the free energy [4, 6, 7]

$$f_\infty(\beta, h) = -2 \int_{\theta_{\text{YL}}(\beta)}^\pi \frac{\theta}{h^2 + \theta^2} G_\infty(\beta, \theta) d\theta. \quad (10)$$

The magnetic susceptibility  $\chi_\infty$  is given by the second derivative of the free energy with respect to  $h$ . Following [4, 6, 7], this leads to

$$G_\infty(\beta, \theta) = \chi_\infty(\beta) (\theta_{\text{YL}}(\beta))^2 \Phi\left(\frac{\theta}{\theta_{\text{YL}}(\beta)}\right), \quad (11)$$

$\Phi(x)$  being some function of  $x$  such that  $\Phi(|x| \leq 1) = 0$ . From (10) and the fact that  $G(\theta_{\text{YL}}, \beta) = 0$ , one gets the specific heat

$$C_{\infty}(\beta) = \left. \frac{\partial^2 f_{\infty}(\beta, h)}{\partial \beta^2} \right|_{h=0} = -2 \int_{\theta_{\text{YL}}(\beta)}^{\pi} \theta^{-1} \frac{d^2 G_{\infty}(\theta, \beta)}{d\beta^2} d\theta. \quad (12)$$

The above formulae are quite general and hold for any model provided it obeys the Lee–Yang theorem.

To proceed further we insert the (model-specific) critical behaviour. Instead of (3) and (4), assume now the following modified critical behaviour for the singular parts of the zero field susceptibility and the specific heat for  $t \gtrsim 0$ .

$$\chi_{\infty} \sim \xi_{\infty}^{2-\eta} t^r, \quad C_{\infty} \sim \xi^{\tilde{\alpha}} t^q. \quad (13)$$

Similarly, assume that the leading scaling behaviour of the Yang–Lee edge in terms of the reduced temperature is

$$\theta_{\text{YL}}(t) \sim \xi^{\lambda} t^p. \quad (14)$$

For  $t \gtrsim 0$  the critical indices are independent of  $t$  [1]. The scaling behaviour of  $C_{\infty}$  can be related to that of  $\chi_{\infty}$  and  $\theta_{\text{YL}}$  through (11) and (12). These give

$$\xi(t)^{\tilde{\alpha}} t^q \propto \xi(t)^{2-\eta+2\lambda} t^{2p+r-2-2\nu}.$$

Therefore,

$$\lambda = \frac{1}{2}(\tilde{\alpha} - 2 + \eta), \quad (15)$$

$$p = \frac{1}{2}(q - r) + 1 + \nu. \quad (16)$$

**Finite-Size Scaling** The finite-size scaling (FSS) hypothesis, first formulated in 1972 by Fisher [8], is a relationship between the scaling behaviour of thermodynamic quantities in the infinite volume limit and the size dependence of their finite volume counterparts. The general statement of FSS, which is expected to hold in all dimensions including the upper critical one [9] is that if  $P_L(t)$  is the value of some thermodynamic quantity  $P$  at reduced temperature  $t$  measured on a system of linear extent  $L$ , then

$$\frac{P_L(0)}{P_{\infty}(t)} = \mathcal{F}_P \left( \frac{\xi_L(0)}{\xi_{\infty}(t)} \right), \quad (17)$$

where  $\xi_L(t)$  is the correlation length of the finite-size system. Luck has shown that, for the  $XY$ -model in two dimensions,  $\xi_L(0)$  is proportional to  $L$  [10]. Fixing the scaling variable, one has

$$\xi_{\infty}(t) \sim x^{-1} L,$$

and from (2)

$$t \sim (\ln L)^{-\frac{1}{\nu}},$$

for large enough  $L$ . Therefore FSS for the susceptibility and the Yang–Lee edge is

$$\chi_L(0) \sim L^{2-\eta} (\ln L)^{-\frac{r}{\nu}}, \quad (18)$$

$$\theta_1(0) \sim L^{\lambda} (\ln L)^{-\frac{p}{\nu}}. \quad (19)$$

For the finite size system it is convenient to consider the zeroes in the complex  $h$ -plane. The singular part of the free energy corresponds to

$$f_L(t, h) = L^{-d} \sum_j \ln(h - i\theta_j(t)) \quad (20)$$

where  $\theta_1 = \theta_{YL}$ . The (reduced) magnetic susceptibility is therefore

$$\chi_L(t) = \left. \frac{\partial^2 f_L}{\partial h^2} \right|_{h=0} = -L^d \sum_j \frac{1}{\theta_j^2}. \quad (21)$$

The lowest lying zeroes are expected to scale in the same way [11] so that

$$\chi_L(t) \propto -L^{-d} \theta_1(t)^{-2}. \quad (22)$$

From (18) and (19) we have

$$L^{2-\eta} (\ln L)^{-\frac{r}{\nu}} \sim L^{-d-2\lambda} (\ln L)^{\frac{2p}{\nu}}, \quad (23)$$

and conclude

$$\tilde{\alpha} = -d, \quad q = -2(1 + \nu). \quad (24)$$

Thus the scaling behaviour of the singular part of the specific heat indeed exhibits multiplicative logarithmic corrections. Accepting the KT predictions  $\nu = 1/2$ ,  $\eta = 1/4$  for  $t \gtrsim 0$ , the leading critical exponent for the Yang-Lee edge  $\lambda$  and the correction exponents  $q$  and  $p$  are

$$\lambda = -\frac{15}{8}, \quad q = -3, \quad p = -\frac{r}{2}. \quad (25)$$

The above analytic considerations have yielded no information on the odd correction exponent  $r$ . The original renormalisation group analysis of Kosterlitz and Thouless [1], in fact, implicitly contained the prediction

$$r = -1/16 \quad (26)$$

as noted by [12]. Subsequent analysis have concentrated on the  $r = 0$  form of the scaling behaviour (18) and the verification that  $\eta(\beta_c) = 1/4$ . Allton and Hamer [13] have conjectured that the deviation of their determination of  $\eta$  from  $1/4$  might be due to logarithmic corrections.

The study of the full scaling form and the numerical determination of  $r$  is the subject of what follows.

**Numerical Procedures** Numerical methods were used to test the scaling picture of the last section. Specifically, we analysed the FSS behaviour of the Yang-Lee edge so as to test the prediction (19), (25)

$$\theta_1(\beta_c) \sim L^\lambda (\ln L)^r. \quad (27)$$

In particular, we sought to confirm  $\lambda = 15/8$  for the leading behaviour and to check if  $r \neq 0$ .

An algorithm based on that of Wolff [14] was used to simulate the XY-model at zero magnetic field ( $h = 0$ ) on square lattices of sizes  $L = 32, 64, 128$  and  $256$ . The values of  $\beta$  at which the simulations took place ( $\beta_o$ ) were evenly spaced in steps of  $0.02$  between  $1.00$  and  $1.20$ . At each

simulation point, 50,000 measurements were made from each of two separate starts. The second runs were used only to verify equilibration and to improve our understanding of the statistical errors. The latter were estimated using bootstrap as described below. The autocorrelation time of the susceptibility was also monitored. Histogram reweighting [15] was used to enable extrapolation between  $\beta_o$  values.

The determination of  $\beta_c$  is inextricably bound up with the assumed critical scaling behaviour. For the present purposes, we adopted a two-stage strategy: we used estimates of  $\beta_c$  from our own and other analyses which had assumed *no* logarithmic corrections then tested the stability of these conclusions with respect both to uncertainties in  $\beta_c$  and to the form of the scaling assumption.

One simple estimate was based on assumed conventional ( $r = 0$ ) scaling of the susceptibility (3). A generalised [16] Roomany-Wyld approximant [17] was used to give estimates of the corresponding renormalisation group beta function for each pair of lattice sizes related by factor of two scaling:

$$\beta_L^{RW} = \left(\frac{2}{\beta^2}\right) \frac{\eta - 2 + 2r \ln(\frac{\ln 2L}{\ln L}) / \ln 2 + \ln(\chi_{2L}/\chi_L) / \ln 2}{\frac{\partial}{\partial \beta} [\chi_{2L}\chi_L]}. \quad (28)$$

A preliminary estimate, using  $\eta = 1/4$  and  $r = 0$ , leads to  $\beta_c = 1.11(1)$  which is at the lower end of the range of published estimates [12], [18], [19]. These span 1.11 to 1.13. The most recent high precision result is 1.1197(5) [19].

**Determination of Lee–Yang Zeroes** When the external field is complex ( $h = h_r + ih_i$ ), the partition function (1) can be rewritten

$$Z_L(\beta, h_r + ih_i) = \text{Re}Z_L(\beta, h_r + ih_i) + i\text{Im}Z_L(\beta, h_r + ih_i), \quad (29)$$

where

$$\begin{aligned} \text{Re}Z_L(\beta, h_r + ih_i) &= \frac{1}{\mathcal{N}} \sum_{\{\vec{\sigma}_x\}} e^{\beta S + h_r M} \cos(h_i M), \\ &= Z_L(\beta, h_r) \langle \cos(h_i M) \rangle_{\beta, h_r}, \end{aligned} \quad (30)$$

and

$$\begin{aligned} \text{Im}Z_L(\beta, h_r + ih_i) &= \frac{1}{\mathcal{N}} \sum_{\{\vec{\sigma}_x\}} e^{\beta S + h_r M} \sin(h_i M), \\ &= Z_L(\beta, h_r) \langle \sin(h_i M) \rangle_{\beta, h_r}. \end{aligned} \quad (31)$$

According to the Lee–Yang theorem the zeroes are on the imaginary  $h$ -axis ( $h_r = 0$ ) where  $\langle \sin(h_i M) \rangle_{\beta, h_r}$  vanishes and so the Lee–Yang zeroes are simply the zeroes of

$$\text{Re}Z_L(\beta, ih_i) \propto \langle \cos(h_i M) \rangle_{\beta, 0}. \quad (32)$$

Thus the Lee–Yang zeroes are easily found. Moreover, one can find them at any  $\beta$  using reweighting techniques [15]. For the lowest lying zeroes at  $\beta = 1.11$  we found  $\theta_1(L) = 0.0023353(7)$ ,  $0.0006350(2)$ ,  $0.00017278(5)$  and  $0.000047062(13)$  for  $L = 32, 64, 128$  and  $256$  respectively. Errors were calculated using the bootstrap method where the data for each  $\beta_o$  are resampled 100

times (with replacement) leading to 100 estimates for  $\theta_1$ , from which the variance and bias can be calculated.

In figure 1 we plot the logarithm of the position of the first Lee–Yang zero against the logarithm of the lattice size  $L$ , at  $\beta = 1.11$ . In the absence of any corrections, the slope should give the leading power-law exponent  $\lambda$ . In fact the slope is  $-1.8776(2)$ , the deviation from the KT value of  $-15/8 = -1.875$  being attributed to the presence of logarithmic corrections. To identify these, and the correction exponent  $r$  in (27),  $\ln(\theta_1 L^{15/8})$  is plotted against  $\ln \ln L$  in figure 2. A straight line is identified. Its slope is  $-0.012(1)$  giving evidence for a non-zero value of  $r$ , albeit not in agreement with the RG predictions of  $-1/16 = -0.0625$  from [1].

At this point, one must investigate the extent to which these conclusions regarding the existence of multiplicative logarithmic corrections depend upon the measurement of  $\beta_c$ . We have attempted to do this systematically by studying the above  $\ln \ln L$  fits for  $r$  as a function of the assumed critical beta. Fits with a range of values of  $r$  (including zero) are possible but not all with acceptable  $\chi^2/\text{degree of freedom}$ . To be conservative, we take ‘acceptable’ to mean less than 2. This corresponds to a minimum confidence level of 14%. In figure 3 we show that acceptable values of  $\chi^2$  are possible only for  $1.110 \lesssim \beta_c \lesssim 1.120$ . The  $r = 0$  solution would correspond to  $\beta_c \approx 1.105$  and  $\chi^2/\text{dof} \approx 4$ . Similarly, we find that a fit with  $r = -1/16$  would correspond to  $\beta_c \approx 1.138$  and  $\chi^2/\text{dof} \approx 16$ .

In summary, assuming the Kosteritz-Thouless value  $\eta = 1/4$ , we find non-zero logarithmic corrections to scaling and a corresponding estimate of the critical temperature:

$$r = -0.023 \pm 0.010, \quad \beta_c = 1.115 \pm .005. \quad (33)$$

As a cross check, one may use the above values for  $r$  and  $\eta$  to find the Roomany-Wyld approximant (28) and estimate  $\beta_c$  from its zeroes. We find  $\beta_c = 1.115 \pm 0.004$  in good agreement with the above. However, we emphasize the much higher precision available to an analysis based on Lee–Yang zeroes rather than on the spin susceptibility.

**Conclusions** Theoretical arguments concerning the consistency of the scaling behaviour of odd and even thermodynamic functions at a KT phase transition have been presented. The generally used scaling formulae have to be modified by multiplicative corrections. These are identified analytically for the specific heat and numerically for the susceptibility. This numerical identification comes via an analysis of Lee–Yang zeroes, the FSS of which is linked to that of the susceptibility.

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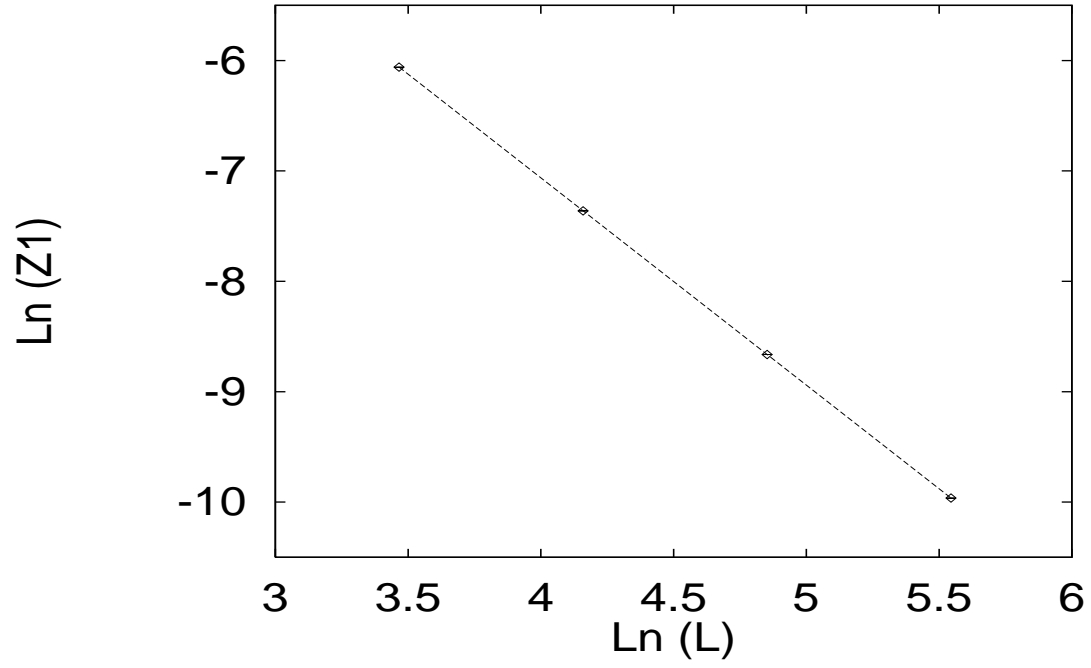


Figure 1: Leading FSS of Lee-Yang Zeroes at  $\beta = 1.11$ .

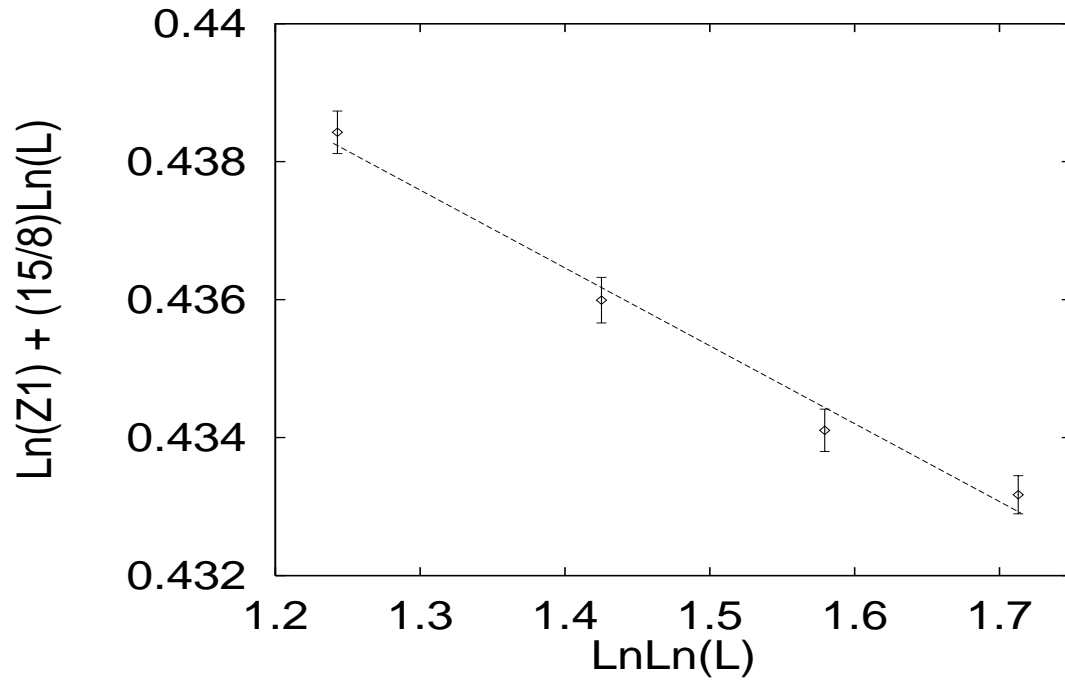


Figure 2: Corrections to FSS of Lee-Yang Zeroes at  $\beta = 1.11$ .

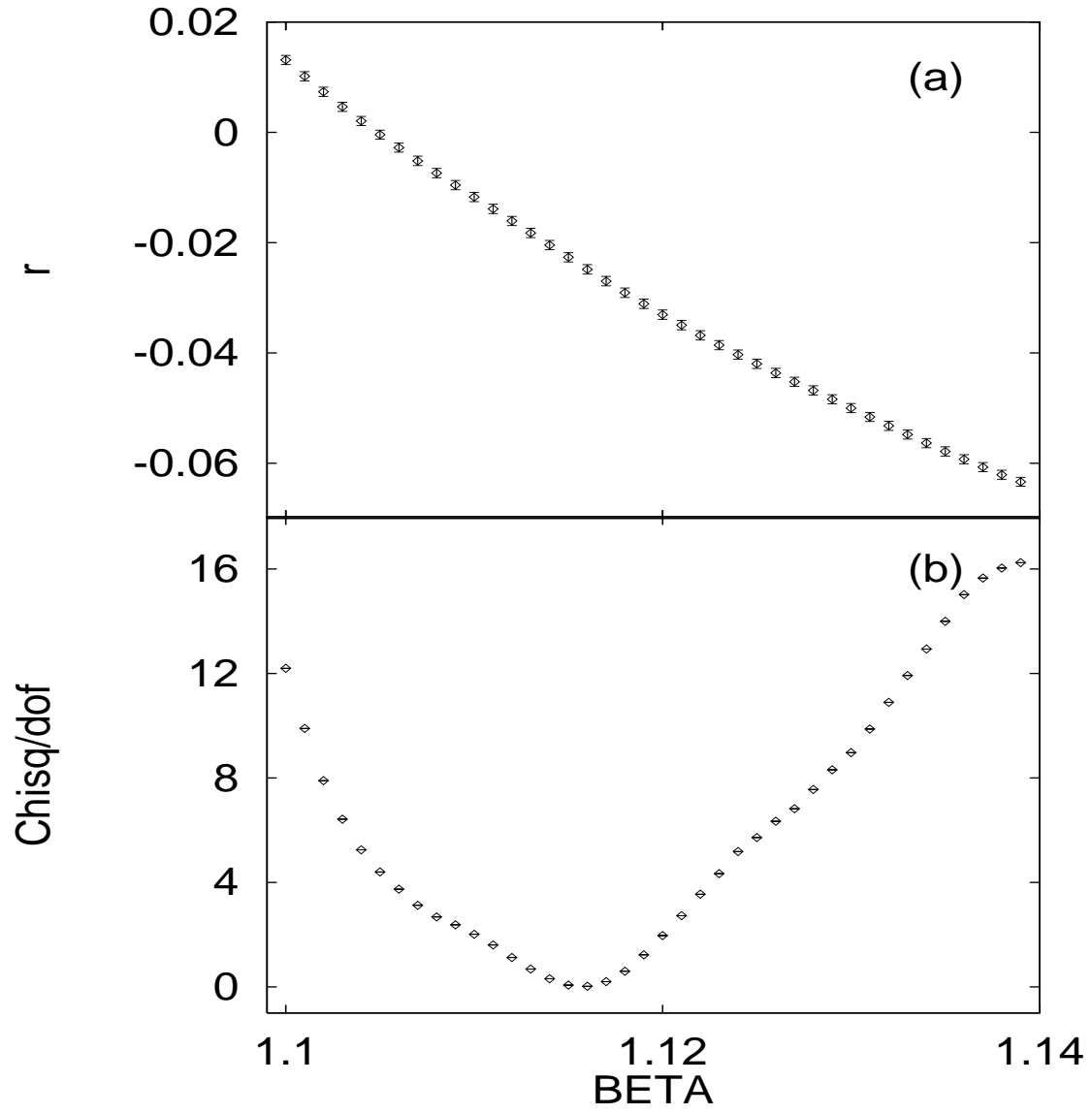


Figure 3: (a) Correction Exponent  $r$  Measured over a Range of  $\beta$  and (b) corresponding  $\chi^2$  per Degree of Freedom (Goodness of Fit).